

Neutron Scattering by Superfluid He II about Dispersion Minimum

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Abstract

We derive the structure factor for superfluid He II about the energy dispersion minimum 1.93 1/\AA .

*This e-print version (2) contains fuller list of the earlier reports on the new superfluid theory.

1 Introduction

For the superfluid described as consisting of a disordered collection of localized atoms[1, 2], the total scattering function may be written in analogy to that of a harmonic solid:

$$S(q, \omega) = S(q) + S_{\text{ph}} + S_{2\text{ph}} + \dots \quad (1)$$

There are of course basic distinctions between $S(q, \omega)$ for the superfluid and for solids, as will be commented where relevant. In the present article, within the framework of the microscopic theory of superfluid He II[1, 2], we derive an expression for the (static) structure factor, the first term $S(q)$ of (1), for the superfluid in the vicinity of $q_b = 1.93 \text{ 1/\AA}$ at which the measured phonon excitation spectrum $\omega(q)$ presents a minimum.

$S(q)$ generally describes the zero-phonon scattering of neutrons, i.e. the scattering processes which do not produce *harmonic* displacement of the superfluid atoms. Denoting the associated atomic displacement in the absolute coordinate system by $u(q)$, then $u(q_b) = 0$. Any scattering involving $u(q) \neq 0$ will yield phonons in a harmonic system, and is accounted for by the higher order "moments" in (1). As we will justify below, $S(q)$ may write as a sum of two terms:

$$S(q) = \frac{1}{2\pi\hbar} e^{-2W} \sum_{l,l'} e^{i\mathbf{q} \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)]} \int e^{-i\omega t} dt [f_0 e^{i0} + f_b e^{i2\pi}] \quad (\text{a})$$

$$= S_0^{\text{el}}(q) + S_b^{\text{inel}}(q) \quad (\text{b}) \quad (2)$$

Where W is Debye-Waller factor; $\mathbf{R}_l(t)$ is the equilibrium position of nucleus l at time t ; the nucleus' displacement from \mathbf{R}_l is \mathbf{u}_l . The "partial" structure factors,

$S_0^{\text{el}}(q)$ and $S_b^{\text{inel}}(q)$, describe an elastic and inelastic scattering, respectively, with the corresponding scattered neutrons undergoing a phase change of zero and of 2π . The subscripts 0 and b indicate the momentum changes the incident neutron undergo are 0 and q_b . f_0 and f_b measure the fractions of the two kinds of scattering events, and satisfy $f_0 + f_b = 1$. The first terms usually presents with harmonic solids, whilst the second term is specific with the superfluid scattering.

2 Elastic scattering of neutrons about q_b

$S_0^{\text{el}}(q)$ of (2b) corresponds to the first summation term of (2a):

$$S_0^{\text{el}}(q) = \frac{1}{2\pi\hbar} e^{-2W} \sum_{l,l'} e^{i\mathbf{q} \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)]} f_0 \int e^{-i\omega t} dt e^{i0} \quad (3)$$

(3) describes an elastic scattering of the neutron, i.e. the momentum of the neutron upon scattering may undergo a change in direction only but not in magnitude. The superfluid atoms are accordingly not produced with any displacement or energy change. The associated phase change on the time axis is thus zero, as is represented by the exponential term e^{i0} .

As is contrasted to a normal liquid which does not give truly elastic scattering except at $q = 0$, the superfluid has the scheme for causing elastic scattering. This is because the energy levels of the superfluid are quantized, as can be satisfactorily accounted for by a SHM (simple harmonic motion)-RSB (relative to superfluid block) dynamics scheme[1]. A momentum transfer will thus not be accompanied with an energy transfer (the case of elastic scattering) unless it equals exactly the energy of a phonon. By contrast, in a normal liquid, the atoms can assume an energy over a continuous range at a given q , so a momentum transfer can always be accompanied by an energy transfer.

For a disordered system, the superfluid here, the site summation in (3), and similarly in (6) below, has the well-known result

$$\sum_{l,l'} e^{i\mathbf{q} \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)]} = N[1 + \int g(R) e^{i\mathbf{q} \cdot \mathbf{R}} dR] \quad (4)$$

where $\mathbf{R} = \mathbf{R}_l(t) - \mathbf{R}_{l'}(0)$. The time integration in (3) yields

$$\int e^{-i(\omega-0)t} dt = \delta(\omega - 0) \quad (5)$$

Substituting (4) and (5) into (3), we have the explicit expression

$$S_0^{\text{el}}(q) = \frac{N}{2\pi\hbar} e^{-2W} \left[1 + \int g(R) e^{i\mathbf{q} \cdot \mathbf{R}} dR \right] f_0 \delta(\omega - 0) \quad (3)'$$

In the elastic scattering here, the neutrons do not directly probe the many-quantum-atom correlation in the superfluid. Instead the neutrons will see the instantaneous

atomic configurations in the liquid, dominated by two factors: (1) the equilibrium positions of the superfluid are short-range disordered, and (2) at each moment in time the atoms are thermally irregularly displaced to instantaneous positions from their equilibrium positions. The thermal displacement of the helium atoms is particularly large owing to their small mass; this is reflected by a large exponent W in the Debye-Waller factor in (3)'. The particularly large atomic displacement in He II, which does not present in normal fluids and harmonic solids with larger atomic masses, determines a particularly broad peak in $S_0^{\text{el}}(q)$, and subsequently in $S(q)$, of the superfluid. This provides an explanation why the structure factor of the superfluid, as revealed from scattering measurements, is abnormally smeared (see e.g. [1]),

The atomic bonding energy of a solid is typically in the range 1–10 eV, which is much greater than the thermal neutron energy E_{ne} (5 – 100 meV). Thus the atomic bonds cannot be broken up (or excited) by the impingement of a thermal neutron. This process is described by $S_b^{\text{inel}}(q)$ to be discussed in Sec. 3. Hence, for a harmonic solid, $S_b^{\text{inel}}(q) = 0$; so $S_0^{\text{el}}(q)$ given in (1) is practically the only term in the structure factor of (2), that is:

$$S^{\text{solid}}(q) = S_0^{\text{el}}(q). \quad (2a)$$

If the solid is also crystalline, then (2a) describes a Bragg scattering, i.e. $S^{\text{solid}}(q) \propto \delta(q - q_b)$.

3 Inelastic scattering at q_b . The superfluid bond excitation

For the superfluid, the atomic bonding energy, being -7.2 K/atom (0.62 meV), is $\ll E_{\text{ne}}$. The superfluid bond can therefore be easily broken up by the impingement of a thermal neutron; one thus expects inelastic neutron scattering to occur at q_b , corresponding to the excitation of the superfluid bond. We actually obtained this through the solution of equation of motion in Ref. [1]. The theoretical anticipation agrees with observation from the thermal neutron measurement, namely that at q_b the neutron energy transfer is finite, and is 8.6 K.

Given that an excitation has occurred and the particle wave has evolved with time, the phase change on the time axis will be non-zero, and this, as we will clarify below, is represented by the second partial structure factor in (2). That is:

$$S_b^{\text{inel}}(q) = \frac{1}{2\pi\hbar} e^{-2W_q} \sum_{l,l'} e^{i\mathbf{q} \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)]} f_b \int e^{i2\pi} e^{-i\omega t} dt \quad (6)$$

We below express the respective terms of (6) explicitly for the present inelastic scattering at q_b , and prove that the phase factor $e^{i2\pi}$ results from the superfluid bond excitation.

Firstly, the Debye-Waller factor at q_b may be evaluated ordinarily to be:

$$W_q|_{q=q_b} = \frac{1}{2} q_b^2 < u >^2 = 0. \quad (7)$$

We next carry out the site summation. As just recalled, the neutron scattering at q_b involves an energy transfer, Δ_s . In such a scattering process a neutron directly communicates with—or probes—the many-quantum-atom correlation in the superfluid. The many-body nature leads to an excellent averaging effect to the fluctuation in cage size and atomic bonding strength in the superfluid over time and locations, yielding an average fluid structure as effectively seen by the scattered neutron. This hence structurally prepares for the neutron scattering intensity to satisfy at q_b the Bragg condition:

$$q_b \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)] = q_b \cdot \mathbf{R} = q_b n a = n 2\pi, \quad n = 0, 1, \dots \quad (8)$$

where a is the apparent interatomic spacing defined by $a = 2\pi/q_b$. It can be readily justified that [1] the Bragg condition (8) indeed holds to a high degree of approximation for the superfluid also according to the relation for neutron's wavevectors before and after scattering, which owing to the inelastic scattering suffers a change that is however negligibly small. With (8), the site summation in (6) writes:

$$\sum_{l,l'} e^{i\mathbf{q} \cdot [\mathbf{R}_l(t) - \mathbf{R}_{l'}(0)]} = \delta(q - q_b). \quad (9)$$

We lastly derive the phase factor $e^{i2\pi}$ of (6). The N -particle system before and after a scattering event is in terms of its macroscopic property unchanged, despite the local perturbation taking place. The total wave functions of the N identical bosonic particles (which solution is given in [1]) before and after the scattering must therefore be the same. For the N boson particle system, this implies that the total phase change of the wave function due to the superfluid bond excitation must satisfy:

$$\text{total phase change} = n' 2\pi \quad (10)$$

n' being integer. The total phase change is a consequence of the evolution of the scattering system in both space and time. As shown by (8), however, the phase change due to the evolution along the X axis, i.e. $q_b a$, alone satisfies 2π . Then, subtracting (8) from (10) gives that the phase change associated with time evolution must alone also satisfy integer times 2π , denoting $n'' 2\pi$. $n'' = 1$ gives the smallest finite phase change and corresponds to one-superfluid bond excitation:

$$0 \xrightarrow{\text{superfluid bond activation}} \frac{\Delta_s}{\hbar} \tau_b = 2\pi, \quad (11)$$

The corresponding contribution to the scattering function is then

$$e^0 \xrightarrow{\text{superfluid bond activation}} e^{\frac{\Delta_s}{\hbar} \tau_b} = e^{i2\pi} \quad (12)$$

The presence of a phase factor $e^{i2\pi}$ in (6), as finally derives from (12), is thus proven.

Substituting (7), (9) and (12) into (6), we obtain the explicit expression for the partial structure factor of the superfluid due to the inelastic scattering of neutrons

at q_b , upon the creations of one-superfluid bonds:

$$\begin{aligned} S_b^{\text{inel}}(q) &= \frac{1}{2\pi\hbar N} \delta(q - q_b) f_b \int_{-\infty}^{\infty} e^{-i(\omega - \frac{\Delta_s}{\hbar})t} \delta(\tau_b) dt \\ &= \frac{1}{2\pi\hbar N} \delta(q - q_b) f_b \delta(\omega - \frac{\Delta_s}{\hbar}) \end{aligned} \quad (6)'$$

Since for the given $q = q_b$, $\omega(q) = \Delta_s/\hbar$. Thus the function $S_b^{\text{inel}}(q)$ at q_b also represents the scattering function at a single point on the ω axis. That is,

$$S_b^{\text{inel}}(q)|_{q=q_b} = S_b(q, \omega)|_{\omega=\frac{\Delta_s}{\hbar}} \quad (13)$$

$S_b(q, \omega)|_{\omega=\frac{\Delta_s}{\hbar}}$ represents $S(q, \omega)$ in the vicinity of (q_b, Δ_s) ; we shall not elaborate on $S(q, \omega)$ in this article.

The excitation energy $\omega = \Delta_s$ at q_b is basically well-defined, or single-valued as a result that Δ_b is single-valued due to the many-quantum-atom correlation in the superfluid as discussed earlier. It follows that the peak in $S_b^{\text{inel}}(q, \omega)|_{\omega=\frac{\Delta_s}{\hbar}}$ will be qualitatively sharp. This provides an explanation of the qualitatively sharp peak feature in $S(q, \omega)$ vs. ω at $q = q_b$, as observed in the inelastic neutron scattering experiments; an actually finite broadening in the peak at q_b can be argued attributable to the finite spreading in δ_s .

4 The total structure factor of the superfluid

Substituting (3)' and (6)' into (2) we finally have the structure factor of the superfluid

$$S(q) = f_0 N \left[1 + \int g(R) e^{i\mathbf{q} \cdot \mathbf{R}} dR \right] \delta(\omega - 0) + f_b \frac{1}{2\pi\hbar N} \delta(q - q_b) \delta(\omega - \frac{\Delta_s}{\hbar}) \quad (2)'$$

Since the two component functions of (2), $S_0^{\text{el}}(q)$ and $S_b^{\text{inel}}(q)$ as explicated in (2)', represent two qualitatively distinct scattering processes, their peak positions do not necessarily coincide. On the q axis, as we surveyed in [1] elastic neutron measurements directly show a peak in $S(q)$ positioned at $q'_b = 2 \text{ \AA}^{-1}$, corresponding to a reciprocal $a' = 2 \text{ \AA}$. From the theoretical representation above we see that this peak is predominately correlated to the elastic scattering process underlying $S_0^{\text{el}}(q)$, i.e. it corresponds to the peak in $S_0^{\text{el}}(q)$. The maximum of $S_b^{\text{inel}}(q)$ is not directly revealed in the measured $S(q)$ v.s q curve. However, on the $\omega(q_b)$ axis inelastic scattering experiments show a minimum of $S(q, \omega)$ positioned at $\omega(q_b)$. If fixing $\omega = \omega(q_b)$ and plotting the function $S_b(q, \omega(q_b)) = S_b^{\text{inel}}(q)$ on the q axis, one would expect a peak position at $q_b = 1.93 \text{ \AA}^{-1}$, which does not coincide with q'_b . This peak at q_b is presumably owing to its weak intensity not directly visible in the measured curve $S(q)$.

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